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Lattice relaxation in α -iron containing small xenon-vacancy clusters

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Binding energies and atomic configurations for small xenon-vacancy clusters in α -iron have been computed using a model based on a two-body potential between the interacting atoms. Various clusters were placed near the center of a sphere containing about 150 iron atoms initially at regular positions in bcc configuration. The results of these calculations are of importance for the interpretation of hyperfine interaction measurements on implanted radioactive sources.

I. INTRODUCTION

Extensive and detailed calculations have been carried out for the binding energies, activation energies, and for atomic configurations around point defects^{1,2} in copper and iron. In all these calculations the two-body forces between atoms in a crystallite containing 100 to 1000 atoms are treated explicitly. Starting with a regular configuration around a point defect, an iteration procedure is followed to find the final atomic configuration, where the net force on the atoms is zero.

Calculations on clusters consisting of one or more xenon atoms and a number of vacancies have been carried out for copper by Anderman and Gehman³ on the same principles as for point defects. In the present paper calculations on small xenon-vacancy clusters in bcc iron are reported. These have been stimulated by the work on the hyperfine interaction of implanted impurities in ferromagnetic and other materials carried out in our laboratory.⁴⁻⁶ The hyperfine interaction results suggest that implanted impurity atoms are located in the host in at most a few different lattice positions and indicate that the impurity atoms may be incorporated in a few types of small and simple clusters, e.g., substitutionally in the host or associated with one or more vacancies. The results of the present calculations have been used for the interpretation of hyperfine interaction studies of radioactive ¹³¹Xe atoms (excited in the decay of ¹³¹I) implanted in Fe.⁷

II. MODEL

The model is the same as that used by Anderman and Gehman³ but we have chosen a considerably smaller crystallite than these authors. In most cases we chose the radius within which the atoms are allowed to move, $R = 5$ lattice units (1 lattice unit = 1.43 Å, the lattice

constant of Fe is 2 lattice units). We placed the cluster under consideration approximately in the center of this sphere. Atoms outside this sphere are kept in fixed positions, which means that the "strength" C of the displacement field² is chosen to be zero outside $R = 5$.

The choice of $R = 5$ is justified by a calculation for the case of a substitutional Xe atom in iron. The formation energies for $R = 5$ and for $R = 4$ are found to differ by less than 1%, showing that $R = 5$ is a sufficiently large radius. The atoms interact through a two-body potential with potential energy $\phi_{ij}(r_{ij})$ between each pair of atoms i and j at a distance r_{ij} . Using the well-known iteration procedure for this type of computation, the end positions of all atoms and the formation energy of the cluster under consideration are calculated.

III. INTERACTION POTENTIALS

For the Fe-Fe interaction potential, $\phi_{Fe}(r)$, we used that of Johnson,² derived from experimental elastic constants. It consists of a composite of three cubic expressions; see Table I. Only first and second neighbors are within the interaction region of an iron atom. The potential represents the short-range ionic interaction only. In transition metals the small long-range electronic interaction was neglected by Johnson. The ratio of distances of first, second and third neighbors in a bcc lattice is $\sqrt{3} : 2 : 2\sqrt{2}$, which justifies the choice of a cutoff distance between the second and third neighbors and the division of elastic-constant data into short-range and long-range contributions.

For the Xe-Xe potential $\phi_{Xe}(r)$ we used a Buckingham potential,^{8,9} $\phi_{Xe}(r) = [\epsilon(1 - 6/\alpha)^{-1}] \{ (6/\alpha) \exp[\alpha(1 - r/r_m)] - (r/r_m)^6 \}$, with $\epsilon = 0.0199$ eV, $r_m = 4.45$ Å, and $\alpha = 13.0$. This potential is found from compressibility and transport properties under conditions where the

TABLE I. Interaction potentials.

Range (lattice units)		Potential (eV)
Fe-Fe potential $\phi_{Fe}(r)$		
1.33	-1.67832	-2.195976(1.43r - 3.097910) ³ + 3.866806r - 7.436448
1.67832	-2.0979	-0.639230(1.43r - 3.115829) ³ + 0.683356r - 1.581570
2.0979	-2.4056	-1.115035(1.43r - 3.066403) ³ + 0.667656r - 1.547967
>2.0456		0
Xe-Fe potential $\phi_{XeFe}(r)$		
1.4	-2.0695	-9.26003(r - 2.14) ³ - 0.665886r + 1.484815
2.0695	-2.48	-1.590333(r - 2.48) ³
≥2.48		0

TABLE II. Vacancy clusters.

Configuration ^a	Formation energy E_n (eV)	Binding energy E_b (eV)		
		This work	Johnson	Beeler
v_1 = one vacancy	2.906
$v_2(1)$ = two vacancies at first nd	5.688	+0.124	+0.13	+0.131
$v_2(2)$ = two vacancies at second nd	5.627	+0.185	+0.20	+0.195
$v_2(3)$ = two vacancies at third nd	5.847	-0.035	...	-0.027
$v_3(112)$ = three vacancies at first and first, and second nd, respectively	8.244	+0.474	...	+0.489
$v_4(111122)$ + Fe = four vacancies + one Fe atom in the center of vacancy tetrahedron	8.899	-0.181

^aIn Tables II and III we used the vacancy-cluster notation of Beeler and Johnson (Ref. 10). The numbers between brackets indicate the pair separation distances involved in the cluster. For example: the notation for two vacancies mutually at first nd (nearest neighbor distance) is $v_2(1)$. The trivacancy $v_3(112)$

involves three vacancies, with pair separation distances first, and first and second (=nearest, nearest and next nearest) neighbor distances. $v_4(111122)$ is a tetravacancy with the largest binding energy, involving four first and two second neighbor distances.

atoms are at somewhat larger distances than in our case.

Following the procedure of Anderman and Gehman,³ an Xe-Fe potential

$$\phi_{\text{XeFe}}(r) = \text{Min} \left\{ \frac{1}{2} [\phi_{\text{Fe}}(2r_{\text{Fe}}) + \phi_{\text{Xe}}(2r_{\text{Xe}})] \right\} \quad (1)$$

is used, r_{Fe} (r_{Xe}) is the radial distance from the center of the Fe atom (Xe atom), $r = r_{\text{Fe}} + r_{\text{Xe}}$ is the distance between the Fe and Xe atom. At a fixed distance r the distances r_{Fe} and r_{Xe} are chosen to minimize the right-hand side of Eq. (1). This minimum is taken as $\phi_{\text{XeFe}}(r)$. In this way we calculated $\phi_{\text{XeFe}}(r)$ for several values of r . An analytic form for the potential was obtained by fitting the numerical data to a sum of cubic relations. The attractive part of the potential, which is very weak, was neglected. The potential, given in Table I, closely resembles a Born-Mayer potential $A \exp(-r/a)$. In the region $2.4 < r < 2.8$ Å the constants have values $A = 7.14 \times 10^3$ eV and $a = 0.281$ Å.

IV. RESULTS FOR VACANCY CLUSTERS

The vacancy configurations studied are given in Table II, together with the computed values of their formation and binding energies. The notation for the various clusters is defined in Table II. The binding energy of a cluster is defined as the total formation

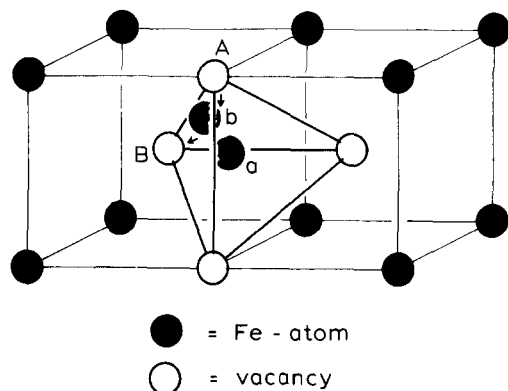


FIG. 1. The vacancy cluster $v_4(111122)$ + Fe. The Fe atom, initially placed at a, travels during 100 iterations to b. The final configuration can be thought as an intermediate state in the vacancy jump from A to B, which is the basic jump in the migration of the trivacancy $v_3(112)$.

energy of the isolated constituents minus the formation energy of the cluster. The binding energy of $v_2(2)$, for instance, is $2E_n(v_1) - E_n(v_2(2)) = 2(2.906) - 5.627 = 0.185$ eV (see Table II). Results of Johnson² and Beeler¹⁰ are also given in Table II.

Since the binding energies found by these authors are not too different from those found by us for a few configurations, we feel that our argument for using a relatively small crystallite is justified.

The cluster $v_4(111122)$ + Fe can be thought of as an intermediate state in the jump of an Fe atom from (000) to (111), or, which is the same, the jump of a vacancy from (111) to (000) (see Fig. 1). This is in fact the basic jump in the process of the migration of the trivacancy $v_3(112)$ from the initial state (111) (020) (11-1) to the final state (000) (020) (11-1). The shape of $v_3(112)$ is not changed in this process. Similar jumps can be made by the other vacancies. In this respect, the difference in binding energy of $v_3(112)$ and $v_4(111122)$ + Fe can be thought of as the (interstitial) migration energy of $v_3(112)$. According to Table II we find 0.655

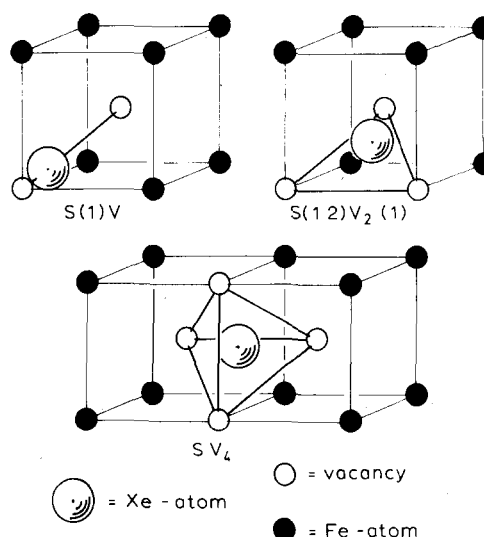


FIG. 2. Schematic final configuration of Xe vacancy clusters. In $s(1)v$ the Xe atom is located at $\sim \frac{1}{4}$ of the distance (000) to (111). In $s(12)v_2(1)$ the Xe atom is roughly in the center of the triangle (000), (111), (200). In sv_4 the Xe atom is roughly in the center of the vacancy tetrahedron.

TABLE III. Xenon-vacancy clusters.

Configuration ^a	Formation energy (eV)	Binding energy (eV)
s = one substitutional Xe atom	8.523	...
$s(1)v$ = one substitutional Xe atom, one vacancy at first nd	10.042	1.387
$s(2)v$ = one substitutional Xe atom, one vacancy at second nd	11.171	0.258
$s(12)v_2(1)$ = one substitutional Xe atom, at first and second nd, two vacancies mutually at first nd	11.275	3.060
$sv_4(111122)$ = one Xe atom in tetrahedron of four vacancies	12.207	5.034
s_2v_{22} = two Xe atoms in hole of 22 vacancies	53.14	27.84

^a See footnote to Table II.

eV for this energy, which is in accordance with the value 0.66 eV found by Beeler and Johnson.¹⁰

V. RESULTS FOR XENON-VACANCY CLUSTERS

A few clusters containing one Xe atom and one cluster containing two Xe atoms were studied. The results for their formation and binding energies and the lattice relaxation, given in Tables III and IV, will be discussed in the following. The notation for the various clusters is defined in Table III. In Table IV we give the equilibrium distances to the Xe atom of a few Fe atoms around these clusters, and in Fig. 2 the equilibrium configuration of three of the Xe-vacancy clusters.

(i) Substitutional Xe atom. The first and second neighbor Fe atoms move outward to positions at a distance 1.89 and 2.07 lattice units from the Xe atom, respectively.

(ii) $s(1)v$. The Xe atom was placed at (000), the vacancy at (111). The Xe atom moves in the direction of the vacancy. In the final configuration the Xe atom has the coordinates (0.247, 0.247, 0.247) and is thus located roughly at $\frac{1}{4}$ of the distance from (000) to (111).

(iii) $s(2)v$. The Xe atom was placed at (000), the vacancy at (200). The Xe atom moves only a distance of 0.07 in the direction of the vacancy.

(iv) $s(12)v_2(1)$. The Xe atom was placed at (000), the vacancies at (111) and (200). The Xe atom moves a large distance; in the equilibrium position it is located roughly in the center of the triangle (000), (111), (200). Thus, this cluster can be viewed as a trivacancy with a Xe atom in the center: $v_3(112) + \text{Xe}$. As mentioned in Sec. IV the trivacancy $v_3(112)$ can migrate without dissociation. Therefore the migration of $s_{12}v_2(1) = v_3(112) + \text{Xe}$ by single vacancy jumps as in the case of $v_3(112)$ could be a mechanism for migration of Xe-vacancy clusters. However, when one more single vacancy meets this cluster the very stable and immobile configuration $sv_4(111122)$ is generated.

(v) $sv_4(111122)$. This cluster resembles the vacancy cluster $v_4(111122) + \text{Fe}$ treated in Sec. IV. Because the Xe-Fe interaction is repulsive we expect the Xe atom to be in equilibrium in the center of the vacancy tetrahedron. This very stable cluster is immobile because it cannot migrate without dissociation. The Xe atom was initially placed a little off the tetrahedron center in

TABLE IV. Relaxation of Fe lattice around $s(1)v$, $s(2)v$, $s(12)v_2(1)$, and $sv_4(111122)$. Original positions of surrounding Fe atoms are given in the second column. The final (equilibrium) distances to the Xe atom are given in the third column. Distances in lattice units.

Configuration	Original position	Final distance to Xe atom
$s(1)v$	(1-11), (11-1), (-111)	1.85
Xe atom originally at (000), vacancy at (111)	(1-1-1), (-1-11), (-11-1)	1.99
Xe atom finally at (0.247, 0.247, 0.247).	(200), (020), (002)	1.94
	(-1-1-1)	2.15
	(-200), (0-20), (00-2) } (220), (202), (022) }	2.54
$s(2)v$	(111), (1-11), (11-1), (1-1-1)	1.87
Xe atom originally at (000), vacancy at (200)	(-111), (-1-11), (-11-1), (-1-1-1)	1.91
Xe atom finally at (0.069, 0, 0)	(020), (0-20), (002), (00-2)	2.08
	(-200)	2.12
$s(12)v_2(1) = v_3(112) + \text{Xe}$, Xe atom originally at (000), vacancies at (111) and (200)	(1-11), (11-1)	1.88
Xe atom finally at (0.994, 0.585, 0.585)	(020), (002)	1.93
	(220), (202)	1.96
	(-111), (311)	2.12
	(022), (222)	2.23
	(1-1-1)	2.19
$sv_4(111122)$. Xe atom initially at (0.45, 0.95, 0.05), vacancies at (000), (111), (11-1), (020)	(-111), (-11-1), (200), (220)	1.96
Final position of Xe atom (0.498, 0.996, 0.0007)	(1-11), (1-1-1), (00-2), (002) } (022), (02-2), (131), (13-1) } (-1-11), (-1-1-1), (-131), (-13-1)	2.29
	(202), (20-2), (222), (22-2)	2.64
	(-200), (-220), (311), (31-1)	2.78
	(113), (11-3), (0-20), (040)	3.09

order to have an asymmetric initial configuration. During 48 iterations the Xe atom moved towards the center.

(vi) s_2v_{22} : In choosing this special cluster we wanted to try a cluster containing two Xe atoms. For the large number of vacancies (22) chosen only a small relaxation of the lattice is expected. Indeed the displacement of the surrounding Fe atoms is only a few percent of a lattice unit. The cluster is a cigar-shaped hole, the Xe atoms were initially placed far off the symmetry line. After a very long run the Xe atoms were nearly on this line.

In Table IV only the distances of a few surrounding Fe atoms to the Xe atom are given. The exact equilibrium positions of many more Fe atoms have been given in an internal report.¹¹

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